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# On a group-theoretical approach to the periodic table of chemical elements

MAURICE R. KIBLER

*Institut de Physique Nucléaire de Lyon  
IN2P3-CNRS et Université Claude Bernard  
43 Bd du 11 Novembre 1918, F-69622 Villeurbanne Cedex, France*

This paper is concerned with the application of the group  $SO(4,2) \otimes SU(2)$  to the periodic table of chemical elements. It is shown how the Madelung rule of the atomic shell model can be used for setting up a periodic table that can be further rationalized via the group  $SO(4,2) \otimes SU(2)$  and some of its subgroups. Qualitative results are obtained from the table and the general lines of a programme for a quantitative approach to the properties of chemical elements are developed on the basis of the group  $SO(4,2) \otimes SU(2)$ .

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*Key words:* hydrogen-like atom, harmonic oscillator, invariance and non-invariance groups, Lie algebra under constraints, Madelung rule, periodic table

## 1 Introduction

Most of the modern presentations of the periodic table of chemical elements are based on a quantum-mechanical treatment of the atom. In this respect, the simplest atom, namely the hydrogen atom, often constitutes a starting point for studying many-electron atoms. Naively, we may expect to construct an atom with atomic number  $Z$  by distributing  $Z$  electrons on the one-electron energy levels of a hydrogen-like atom. This building-up principle can be rationalized and refined from a group-theoretical point of view. As a matter of fact, we know that the dynamical noninvariance group of a hydrogen-like atom is the special real pseudo-orthogonal group in 4+2 dimensions (or conformal group)  $SO(4,2)$  or  $SO(4,2) \otimes SU(2)$  if we introduce the group  $SU(2)$  that labels the spin [1-3]. This result can be derived in several ways. We briefly review two of them.

The first way is quite well-known and corresponds to a symmetry ascent process starting from the geometrical symmetry group  $SO(3)$  of a hydrogen-like atom. Then, we go from  $SO(3)$  to the dynamical invariance group  $SO(4)$  for the discrete spectrum or  $SO(3,1)$  for the continuous spectrum. The relevant quantum numbers for the discrete spectrum are  $n$ ,  $\ell$  and  $m_\ell$  (with  $n = 1, 2, 3, \dots$ ; for fixed  $n$ :  $\ell = 0, 1, \dots, n-1$ ; for fixed  $\ell$ :  $m_\ell = -\ell, -\ell+1, \dots, \ell$ ). The corresponding state vectors  $\Psi_{n\ell m_\ell}$  can be organized to span multiplets of  $SO(3)$  and  $SO(4)$ . The set  $\{\Psi_{n\ell m_\ell} : n \text{ and } \ell \text{ fixed}; m_\ell \text{ ranging}\}$  generates an irreducible representation class (IRC), noted  $(\ell)$ , while the set  $\{\Psi_{n\ell m_\ell} : n \text{ fixed}; \ell \text{ and } m_\ell \text{ ranging}\}$  generates an IRC of  $SO(4)$ . The direct sum

$$h = \bigoplus_{n=1}^{\infty} \bigoplus_{\ell=0}^{n-1} (\ell)$$

spanned by all the possible state vectors  $\Psi_{n\ell m_\ell}$  corresponds to an IRC of the de Sitter group  $\text{SO}(4, 1)$ . The IRC  $h$  is also an IRC of  $\text{SO}(4, 2)$ . This IRC thus remains irreducible when restricting  $\text{SO}(4, 2)$  to  $\text{SO}(4, 1)$  but splits into two IRC's when restricting  $\text{SO}(4, 2)$  to  $\text{SO}(3, 2)$ . The groups  $\text{SO}(4, 2)$ ,  $\text{SO}(4, 1)$  and  $\text{SO}(3, 2)$  are dynamical noninvariance groups in the sense that not all their generators commute with the Hamiltonian of the hydrogen-like atom.

The second way to derive  $\text{SO}(4, 2)$  corresponds to a symmetry descent process starting from the dynamical noninvariance group  $\text{Sp}(8, \mathbf{R})$ , the real symplectic group in 8 dimensions, for a four-dimensional isotropic harmonic oscillator. We know that there is a connection between the hydrogen-like atom in  $\mathbf{R}^3$  and a four-dimensional oscillator in  $\mathbf{R}^4$  [3-4]. Such a connection can be established via Lie-like methods (local or infinitesimal approach) or algebraic methods based on the so-called Kustaanheimo-Stiefel transformation (global or partial differential equation approach). Both approaches give rise to a constraint and the introduction of this constraint into the Lie algebra of  $\text{Sp}(8, \mathbf{R})$  produces a Lie algebra under constraints that turns out to be isomorphic with the Lie algebra of  $\text{SO}(4, 2)$ . From a mathematical point of view, the latter Lie algebra is given by [5]

$$\text{cent}_{\text{sp}(8, \mathbf{R})} \text{so}(2) / \text{so}(2) = \text{su}(2, 2) \sim \text{so}(4, 2)$$

in terms of Lie algebras.

Once we accept that the hydrogen-like atom may serve as a guide for studying the periodic table, the group  $\text{SO}(4, 2)$  and some of its subgroups play an important role in the construction of this table. This was first realized in by Barut [6] and, independently, by Konopel'chenko [7]. Later, Byakov *et al.* [8] further developed this group-theoretical approach of the periodic chart of chemical elements by introducing the direct product  $\text{SO}(4, 2) \otimes \text{SU}(2)$ .

The aim of this paper is to emphasize the importance of a connection between the periodic table *à la*  $\text{SO}(4, 2) \otimes \text{SU}(2)$  and the Madelung rule [9] of atomic spectroscopy. The material is organized as follows. In Section 2, a periodic table is derived from the Madelung rule. In Section 3, this table is rationalized in terms of  $\text{SO}(4, 2) \otimes \text{SU}(2)$ . Some qualitative and quantitative aspects of the table are described in Sections 4 and 5. This paper constitutes a companion article to four previous papers by the author [10].

## 2 The periodic table *à la* Madelung

We first describe the construction of a periodic table based on the so-called Madelung rule [9] which arises from the atomic shell model. This approach to the periodic table uses the quantum numbers occurring in the quantum-mechanical treatment of the hydrogen atom as well as of a many-electron atom.

In the central-field approximation, each of the  $Z$  electrons of an atom with atomic number  $Z$  is partly characterized by the quantum numbers  $n$ ,  $\ell$ , and  $m_\ell$ . The numbers  $\ell$  and  $m_\ell$  are the orbital quantum number and the magnetic quantum number, respectively. They are connected to the chain of groups  $\text{SO}(3) \supset \text{SO}(2)$ : the

quantum number  $\ell$  characterizes an IRC, of dimension  $2\ell + 1$ , of  $\text{SO}(3)$  and  $m_\ell$  a one-dimensional IRC of  $\text{SO}(2)$ . The principal quantum number  $n$  is such that  $n - \ell - 1$  is the number of nodes of the radial wave function associated with the doublet  $(n, \ell)$ . In the case of the hydrogen atom or of a hydrogen-like atom, the number  $n$  is connected to the group  $\text{SO}(4)$ : the quantum number  $n$  characterizes an IRC, of dimension  $n^2$ , of  $\text{SO}(4)$ . The latter IRC of  $\text{SO}(4)$  splits into the IRC's of  $\text{SO}(3)$  corresponding to  $\ell = 0, 1, \dots, n - 1$  when  $\text{SO}(4)$  is restricted to  $\text{SO}(3)$ . A complete characterization of the dynamical state of each electron is provided by the quartet  $(n, \ell, m_\ell, m_s)$  or alternatively  $(n, \ell, j, m)$ . Here, the spin  $s = \frac{1}{2}$  of the electron has been introduced and  $m_s$  is the  $z$ -component of the spin. Furthermore,  $j = \frac{1}{2}$  for  $\ell = 0$  and  $j$  can take the values  $j = \ell - s$  and  $j = \ell + s$  for  $\ell \neq 0$ . The quantum numbers  $j$  and  $m$  are connected to the chain of groups  $\text{SU}(2) \supset \text{U}(1)$ :  $j$  characterizes an IRC, of dimension  $2j + 1$ , of  $\text{SU}(2)$  and  $m$  a one-dimensional IRC of  $\text{U}(1)$ .

Each doublet  $(n, \ell)$  defines an atomic shell. The ground state of the atom is obtained by distributing the  $Z$  electrons of the atom among the various atomic shells  $n\ell, n'\ell', n''\ell'', \dots$  according to (i) an ordering rule and (ii) the Pauli exclusion principle. A somewhat idealized situation is provided by the Madelung ordering rule: the energy of the shells increases with  $n + \ell$  and, for a given value of  $n + \ell$ , with  $n$  [9]. This may be depicted by Fig. 1 where the rows are labelled with  $n = 1, 2, 3, \dots$  and the columns with  $\ell = 0, 1, 2, \dots$  and where the entry in the  $n$ -th row and  $\ell$ -th column is  $[n + \ell, n]$ . We thus have the ordering  $[1, 1] < [2, 2] < [3, 2] < [3, 3] < [4, 3] < [4, 4] < [5, 3] < [5, 4] < [5, 5] < [6, 4] < [6, 5] < [6, 6] < \dots$ . This dictionary order corresponds to the following ordering of the  $n\ell$  shells

$$1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < \dots$$

which is verified to a good extent by experimental data. (According to atomic spectroscopy, we use the letters  $s$  (for sharp),  $p$  (for principal),  $d$  (for diffuse),  $f$  (for fundamental), ... to denote  $\ell = 0, 1, 2, 3, \dots$ , respectively.)

From these considerations of an entirely atomic character, we can construct a periodic table of chemical elements. We start from the Madelung array of Fig. 1. Here, the significance of the quantum numbers  $n$  and  $\ell$  is abandoned. The numbers  $n$  and  $\ell$  are now simple row and column indexes, respectively. We thus forget about the significance of the quartet  $n, \ell, j, m$ . The various blocks  $[n + \ell, n]$  are filled in the dictionary order, starting from  $[1, 1]$ , with chemical elements of increasing atomic numbers. More precisely, the block  $[n + \ell, n]$  is filled with  $2(2\ell + 1)$  elements, the atomic numbers of which increase from left to right. This yields Fig. 2, where each element is denoted by its atomic number  $Z$ . For instance, the block  $[1, 1]$  is filled with  $2(2 \times 0 + 1) = 2$  elements corresponding to  $Z = 1$  up to  $Z = 2$ . In a similar way, the blocks  $[2, 2]$  and  $[3, 2]$  are filled with  $2(2 \times 0 + 1) = 2$  elements and  $2(2 \times 1 + 1) = 6$  elements corresponding to  $Z = 3$  up to  $Z = 4$  and to  $Z = 5$  up to  $Z = 10$ , respectively. It is to be noted, that the so obtained periodic table *a priori* contains an infinite number of elements: the  $n$ -th row contains  $2n^2$  elements and each column (bounded from top) contains an infinite number of elements.

	0	1	2	3	4	...
1	[1,1]					
2	[2,2]	[3,2]				
3	[3,3]	[4,3]	[5,3]			
4	[4,4]	[5,4]	[6,4]	[7,4]		
5	[5,5]	[6,5]	[7,5]	[8,5]	[...]	
6	[6,6]	[...]				
7	[...]					
...						

Fig. 1. The  $[n + \ell, n]$  Madelung array. The lines are labelled by  $n = 1, 2, 3, \dots$  and the columns by  $\ell = 0, 1, 2, \dots$ . For fixed  $n$ , the label  $\ell$  assumes the values  $\ell = 0, 1, \dots, n - 1$ .

	l = 0 (s-block)	l = 1 (p-block)	l = 2 (d-block)	l = 3 (f-block)	l = 4 (g-block)	...
n = 1	1 up to 2					
n = 2	3 up to 4	5 up to 10				
n = 3	11 up to 12	13 up to 18	21 up to 30			
n = 4	19 up to 20	31 up to 36	39 up to 48	57 up to 70		
n = 5	37 up to 38	49 up to 54	71 up to 80	89 up to 102	121 up to 138	
n = 6	55 up to 56	81 up to 86	103 up to 112	139 up to 152	...	
n = 7	87 up to 88	113 up to 118	153 up to 162	...		
n = 8	119 up to 120	163 up to 168	...			
n = 9	169 up to 170	...				
...	...					

Fig. 2. The periodic table deduced from the Madelung array. The box  $[n + \ell, n]$  is filled with  $2(2\ell + 1)$  elements. The filling of the various boxes  $[n + \ell, n]$  is done according to the dictionary order implied by Fig. 1.

### 3 The periodic table à la $\text{SO}(4, 2) \otimes \text{SU}(2)$

We are now in a position to give a group-theoretical articulation to the periodic table of Fig. 2. For fixed  $n$ , the  $2(2\ell + 1)$  elements in the block  $[n + \ell, n]$ , that we shall refer to an  $\ell$ -block, may be labelled in the following way. For  $\ell = 0$ , the  $s$ -block in the  $n$ -th row contains two elements that we can distinguish by the number  $m$  with  $m$  ranging from  $-\frac{1}{2}$  to  $\frac{1}{2}$  when going from left to right in the row. For  $\ell \neq 0$ , the  $\ell$ -block in the  $n$ -th row can be divided into two sub-blocks, one corresponding to  $j = \ell - \frac{1}{2}$  (on the left) and the other to  $j = \ell + \frac{1}{2}$  (on the right). Each sub-block contains  $2j + 1$  elements (with  $2j + 1 = 2\ell$  for  $j = \ell - \frac{1}{2}$  and  $2j + 1 = 2(\ell + 1)$  for  $j = \ell + \frac{1}{2}$ ) that can be distinguished by the number  $m$  with  $m$  ranging from  $-j$  to  $j$  by step of one unit when going from left to right in the row. In other words, a chemical element can be located in the table by the quartet  $(n, \ell, j, m)$  (where  $j = \frac{1}{2}$  for  $\ell = 0$ ).

Following Byakov *et al.* [8], it is perhaps interesting to use an image with streets, avenues and houses in a city. Let us call Mendeleev city the city whose (west-east) streets are labelled by  $n$  and (north-south) avenues by  $(\ell, j, m)$ . In the  $n$ -th street there are  $n$  blocks of houses. The  $n$  blocks are labelled by  $\ell = 0, 1, \dots, n - 1$  so that the address of a block is  $(n, \ell)$ . Each block contains one sub-block (for  $\ell = 0$ ) or two sub-blocks (for  $\ell \neq 0$ ). An address  $(n, \ell, j, m)$  can be given to each house:  $n$  indicates the street,  $\ell$  the block,  $j$  the sub-block and  $m$  the location inside the sub-block. The organization of the city appears in Fig. 3.

At this stage, it is worthwhile to re-give to the quartet  $(n, \ell, j, m)$  its group-theoretical significance. Then, Mendeleev city is clearly associated to the IRC class  $h \otimes [2]$  of  $\text{SO}(4, 2) \otimes \text{SU}(2)$  where  $[2]$  stands for the fundamental representation of  $\text{SU}(2)$ . The whole city corresponds to the IRC

$$\bigoplus_{n=1}^{\infty} \bigoplus_{\ell=0}^{n-1} \bigoplus_{j=|\ell-\frac{1}{2}|}^{j=\ell+\frac{1}{2}} (j) = \left( \bigoplus_{n=1}^{\infty} \bigoplus_{\ell=0}^{n-1} (\ell) \right) \otimes [2]$$

of  $\text{SO}(4, 2) \otimes \text{SU}(2)$  in the sense that all the possible quartets  $(n, \ell, j, m)$ , or alternatively  $(n, \ell, m_\ell, m_s)$ , can be associated to state vectors spanning this IRC. (In the latter equation,  $(\ell)$  and  $(j)$  stand for the IRC's of  $\text{SO}(3)$  and  $\text{SU}(2)$  associated with the quantum numbers  $\ell$  and  $j$ , respectively.)

We can ask the question: how to move in Mendeleev city? Indeed, there are several bus lines to go from one house to another one? The  $\text{SO}(3)$  bus lines (also called  $\text{SO}(3) \otimes \text{SU}(2)$  ladder operators) make it possible to go from one house in a given  $\ell$ -block to another house in the same  $\ell$ -block (see Fig. 4). The  $\text{SO}(4)$  bus lines (also called  $\text{SO}(4) \otimes \text{SU}(2)$  ladder operators) and the  $\text{SO}(2, 1)$  bus lines (also called  $\text{SO}(2, 1)$  ladder operators) allow to move in a given street (see Fig. 5) and in a given avenue (see Fig. 6), respectively. Finally, it should be noted that there are taxis (also called  $\text{SO}(4, 2) \otimes \text{SU}(2)$  ladder operators) to go from a given house to an arbitrary house.

Another question concerns the inhabitants (also called chemical elements) of Mendeleev city. In fact, they are distinguished by a number  $Z$  (also called the

atomic number). The inhabitant living at the address  $(n, \ell, j, m)$  has the number

$$\begin{aligned} Z(n\ell jm) = & \frac{1}{6}(n+\ell)[(n+\ell)^2 - 1] + \frac{1}{2}(n+\ell+1)^2 \\ & - \frac{1}{4}[1 + (-1)^{n+\ell}](n+\ell+1) - 4\ell(\ell+1) + \ell + j(2\ell+1) + m - 1 \end{aligned}$$

Each inhabitant may also have a nickname. All the inhabitants up to  $Z = 110$  have a nickname. For example, we have Ds, or darmstadtium in full, for  $Z = 110$ . Not all the houses in Mendeleev city are inhabited. The inhabited houses go from  $Z = 1$  to  $Z = 116$  (the houses  $Z = 113$  and  $Z = 115$  are occupied since the beginning of 2004 [11]). The houses corresponding to  $Z \geq 117$  are not presently inhabited. (When a house is not inhabited, we also say that the corresponding element has not been observed yet.) The houses from  $Z = 111$  to  $Z = 116$  are inhabited but have not received a nickname yet. The various inhabitants known at the present time are indicated on Fig. 7.

It is not forbidden to get married in Mendeleev city. Each inhabitant may get married with one or several inhabitants (including one or several clones). For example, we know  $\text{H}_2$  (including H and its clone),  $\text{HCl}$  (including H and Cl), and  $\text{H}_2\text{O}$  (including O, H and its clone). However, there is a strict rule in the city: the assemblages or married inhabitants have to leave the city. They must live in another city and go to a city sometimes referred to as a molecular city. (Only the clones can stay in Mendeleev city.)

#### 4 Qualitative aspects of the periodic table

Going back to Physics and Chemistry, we now describe Mendeleev city as a periodic table for chemical elements. We have obtained a table with rows and columns for which the  $n$ -th row contains  $2n^2$  elements and the  $(\ell, j, m)$ -th column contains an infinite number of elements. A given column corresponds to a family of chemical analogs in the standard periodic table and a given row may contain several periods of the standard periodic table.

The chemical elements in their ground state are considered as different states of atomic matter: each atom in the table appears as a particular partner for the (infinite-dimensional) unitary irreducible representation  $h \otimes [2]$  of the group  $\text{SO}(4, 2) \otimes \text{SU}(2)$ , where  $\text{SO}(4, 2)$  is reminiscent of the hydrogen atom and  $\text{SU}(2)$  is introduced for a doubling purpose. In fact, it is possible to connect two partners of the representation  $h \otimes [2]$  by making use of shift operators of the Lie algebra of  $\text{SO}(4, 2) \otimes \text{SU}(2)$ . In other words, it is possible to pass from one atom to another one by means of raising or lowering operators. The internal dynamics of each element is ignored. In other words, each neutral atom is assumed to be a noncomposite physical system. By way of illustration, we give a brief description of some particular columns and rows of the table.

The alkali-metal atoms (see Fig. 8) are in the first column (with  $\ell = 0$ ,  $j = \frac{1}{2}$ , and  $m = -\frac{1}{2}$ ); in the atomic shell model, they correspond to an external shell of type  $1s, 2s, 3s, \dots$ ; we note that hydrogen (H) belongs to the alkali-metal atoms.

The second column (with  $\ell = 0$ ,  $j = \frac{1}{2}$ , and  $m = \frac{1}{2}$ ) concerns the alkaline earth metals (see Fig. 9) with an external atomic shell of type  $1s^2, 2s^2, 3s^2, \dots$ ; we note that helium (He) belongs to the alkaline earth metals. The sixth column corresponds to chalcogens (see Fig. 10) and the seventh column to halogens (see Fig. 11); it is to be observed that hydrogen does not belong to halogens as it is often the case in usual periodic tables. The eighth column (with  $\ell = 1$ ,  $j = \frac{3}{2}$ , and  $m = \frac{3}{2}$ ) gives the noble gases (see Fig. 12) with an external atomic shell of type  $2p^6, 3p^6, 4p^6, \dots$ ; helium (with the atomic configuration  $1s^2 2s^2$ ) does not belong to the noble gases in contrast with usual periodic tables.

The  $d$ -blocks with  $n = 3, 4$  and  $5$  yield the three familiar transition series (see Fig. 13): the iron group goes from Sc(21) to Zn(30), the palladium group from Y(39) to Cd(48) and the platinum group from Lu(71) to Hg(80). A fourth transition series goes from Lr(103) to  $Z = 112$  (observed but not named yet). In the shell model, the four transition series correspond to the filling of the  $nd$  shell while the  $(n+1)s$  shell is fully occupied, with  $n = 3$  (iron group series),  $n = 4$  (palladium group series),  $n = 5$  (platinum group series) and  $n = 6$  (fourth series). The two familiar inner transition series are the  $f$ -blocks with  $n = 4$  and  $n = 5$  (see Fig. 14): the lanthanide series goes from La(57) to Yb(70) and the actinide series from Ac(89) to No(102). Observe that lanthanides start with La(57) not Ce(58) and actinides start with Ac(89) not Th(90). We note that lanthanides and actinides occupy a natural place in the table and are not reduced to appendages as it is generally the case in usual periodic tables in 18 columns. A superactinide series is predicted to go from  $Z = 139$  to  $Z = 152$  (and not from  $Z = 122$  to  $Z = 153$  as predicted by Seaborg [12]). In a shell model approach, the inner transition series correspond to the filling of the  $nf$  shell while the  $(n+2)s$  shell is fully occupied, with  $n = 4$  (lanthanides),  $n = 5$  (actinides) and  $n = 6$  (superactinides). The table in Fig. 7 shows that the elements from  $Z = 121$  to  $Z = 138$  form a new period having no homologue among the known elements.

In Section 3, we have noted that each  $\ell$ -block with  $\ell \neq 0$  gives rise to two sub-blocks. As an example, the  $f$ -block for the lanthanides is composed of a sub-block (corresponding to  $j = \frac{5}{2}$ ) from La(57) to Sm(62) and another one (corresponding to  $j = \frac{7}{2}$ ) from Eu(63) to Yb(70) (see Fig. 15). This division corresponds to the classification in light or ceric rare earths and heavy or yttric rare earths. It has received justifications both from the experimental and the theoretical sides.

## 5 Quantitative aspects of the periodic table

To date, the use of  $SO(4, 2)$  or  $SO(4, 2) \otimes SU(2)$  in connection with periodic charts has been limited to qualitative aspects only, viz., classification of neutral atoms and ions as well. We would like to give here the main lines of a programme under development (inherited from nuclear physics and particle physics) for dealing with quantitative aspects.

The first step concerns the mathematics of the programme. The direct product group  $SO(4, 2) \otimes SU(2)$  is a Lie group of order eighteen. Let us first consider the



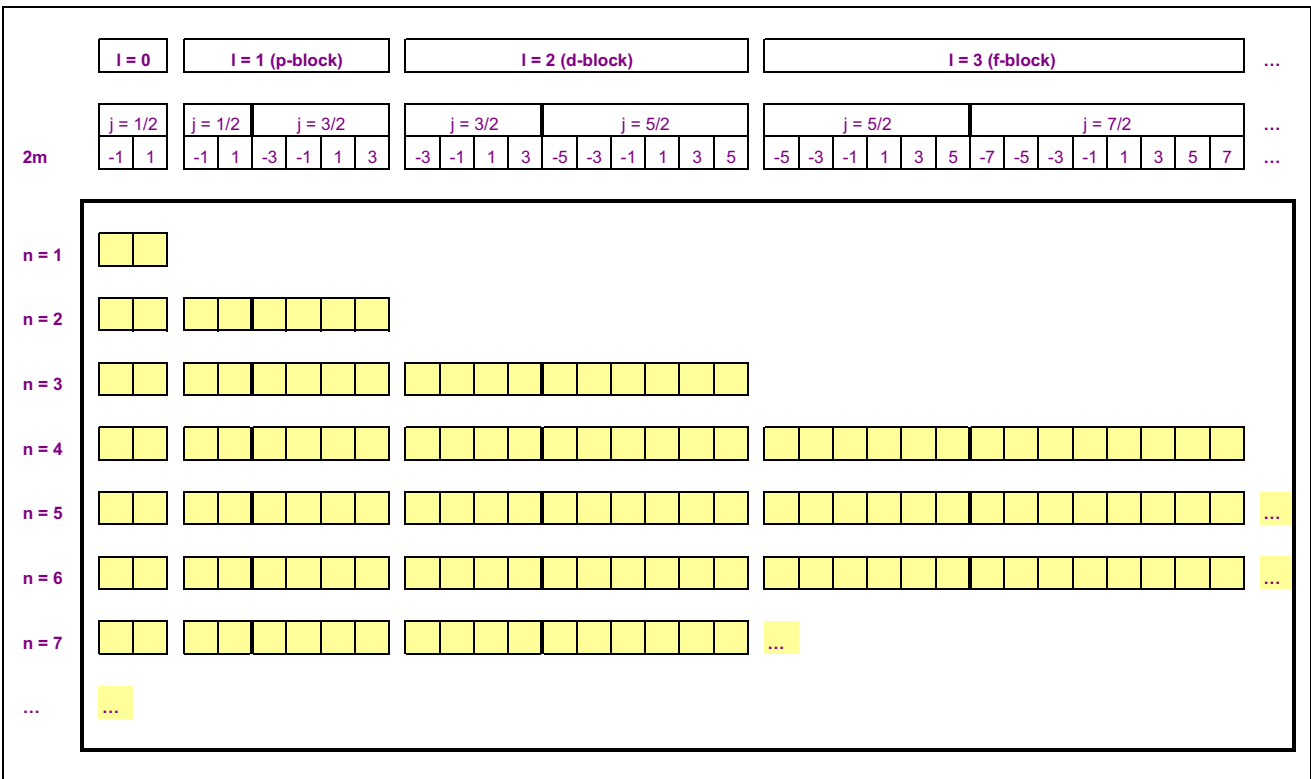


Fig. 3. Mendeleev city. The streets are labelled by  $n \in \mathbf{N}^*$  and the avenues by  $(\ell, j, m)$  [ $\ell = 0, 1, \dots, n-1$ ;  $j = \frac{1}{2}$  for  $\ell = 0$ ,  $j = \ell - \frac{1}{2}$  or  $j = \ell + \frac{1}{2}$  for  $\ell \neq 0$ ;  $m = -j, -j+1, \dots, j$ ].

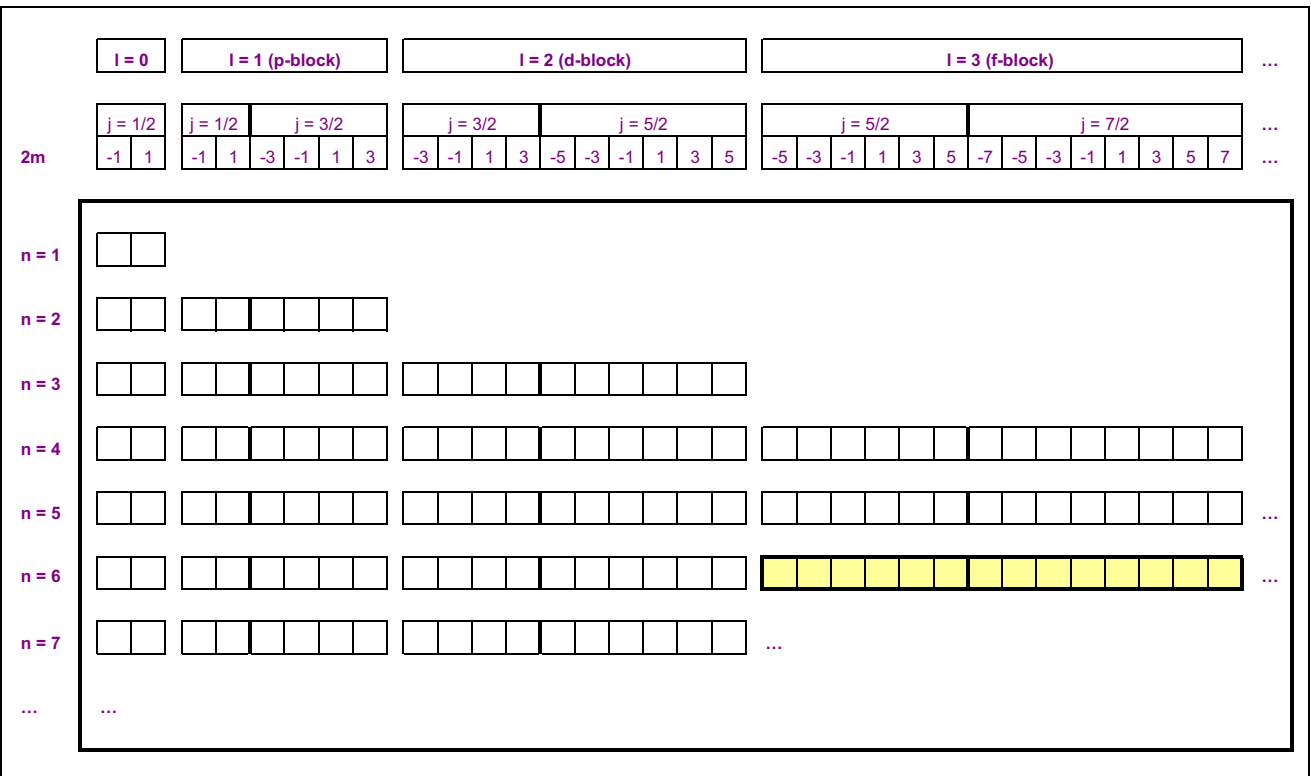


Fig. 4. How to move in Mendeleviev city? To move inside a block, take an  $SO(3) \otimes SU(2)$  bus line! The shaded bus line corresponds to  $\ell = 3$  and  $n = 6$ .



$\mathrm{SO}(2,1)$  bus line! The shaded bus line corresponds to  $\ell = 0$ ,  $j = \frac{1}{2}$ , and  $m = -\frac{1}{2}$ .

1 2 H He										
3 4 Li Be	5 6 B C	7 8 9 10 N O F Ne								
11 12 Na Mg	13 14 Al Si	15 16 17 18 P S Cl Ar	21 22 23 24 Sc Ti V Cr	25 26 27 28 29 30 Mn Fe Co Ni Cu Zn						
19 20 K Ca	31 32 Ga Ge	33 34 35 36 As Se Br Kr	39 40 41 42 Y Zr Nb Mo	43 44 45 46 47 48 Tc Ru Rh Pd Ag Cd	57 58 59 60 61 62 La Ce Pr Nd Pm Sm	63 64 65 66 67 68 69 70 Eu Gd Tb Dy Ho Er Tm Yb				
37 38 Rb Sr	49 50 In Sn	51 52 53 54 Sb Te I Xe	71 72 73 74 Lu Hf Ta W	75 76 77 78 79 80 Re Os Ir Pt Au Hg	89 90 91 92 93 94 Ac Th Pa U Np Pu	95 96 97 98 99 100 101 102 Am Cm Bk Cf Es Fm Md No	121 - 138 no			
55 56 Cs Ba	81 82 Tl Pb	83 84 85 86 Bi Po At Rn	103 104 105 106 Lr Rf Db Sg	107 108 109 110 111 112 Bh Hs Mt Ds X? X?	139 140 141 142 143 144 no no no no no no	145 146 147 148 149 150 151 152 no no no no no no no no	... ...			
87 88 Fr Ra	113 114 X? X?	115 116 117 118 X? X? no no	153 154 155 156 no no no no	157 158 159 160 161 162 no no no no no no	... ...					
... ...										

Fig. 7. The inhabitants of Mendeleev city. The houses up to number  $Z = 116$  are inhabited [‘X?’ means inhabited (or observed) but not named, ‘no’ means not inhabited (or not observed)].

1 H	2 He																																								
3 Li	4 Be	5 B	6 C	7 N	8 O	9 F	10 Ne																																		
11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn																								
19 K	20 Ca	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb										
37 Rb	38 Sr	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	121 - 138 no									
55 Cs	56 Ba	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 X?	112 X?	139 no	140 no	141 no	142 no	143 no	144 no	145 no	146 no	147 no	148 no	149 no	150 no	151 no	152 no	...									
87 Fr	88 Ra	113 X?	114 X?	115 X?	116 X?	117 no	118 no	153 no	154 no	155 no	156 no	157 no	158 no	159 no	160 no	161 no	162 no	...											...												
...	...																																								

Fig. 8. The inhabitants of Mendeleev city. The family of alkali metals (with an infinite number of elements) corresponds to  $(\ell = 0, j = \frac{1}{2}, m = -\frac{1}{2})$  and  $n \in \mathbf{N}^*$ .

1 H	2 He																															
3 Li	4 Be	5 B	6 C	7 N	8 O	9 F	10 Ne																									
11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn															
19 K	20 Ca	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	
37 Rb	38 Sr	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	121 - 138 no
55 Cs	56 Ba	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 X?	112 X?	139 no	140 no	141 no	142 no	143 no	144 no	145 no	146 no	147 no	148 no	149 no	150 no	151 no	152 no	...
87 Fr	88 Ra	113 X?	114 X?	115 X?	116 X?	117 no	118 no	153 no	154 no	155 no	156 no	157 no	158 no	159 no	160 no	161 no	162 no	...											...			
...	...																															

Fig. 9. The inhabitants of Mendeleev city. The family of alkaline earth metals (with an infinite number of elements) corresponds to  $(\ell = 0, j = \frac{1}{2}, m = \frac{1}{2})$  and  $n \in \mathbf{N}^*$ .

1 H	2 He																																								
3 Li	4 Be	5 B	6 C	7 N	8 O	9 F	10 Ne																																		
11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn																								
19 K	20 Ca	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb										
37 Rb	38 Sr	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	121 - 138 no									
55 Cs	56 Ba	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 X?	112 X?	139 no	140 no	141 no	142 no	143 no	144 no	145 no	146 no	147 no	148 no	149 no	150 no	151 no	152 no	...									
87 Fr	88 Ra	113 X?	114 X?	115 X?	116 X?	117 no	118 no	153 no	154 no	155 no	156 no	157 no	158 no	159 no	160 no	161 no	162 no	...									...														
...	...																															...									

Fig. 10. The inhabitants of Mendeleev city. The family of chalcogens (with an infinite number of elements) corresponds to  $(\ell = 1, j = \frac{3}{2}, m = -\frac{1}{2})$  and  $n = 2, 3, 4, \dots$ .



1 H	2 He																																									
3 Li	4 Be	5 B	6 C	7 N	8 O	9 F	10 Ne																																			
11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn																									
19 K	20 Ca	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb											
37 Rb	38 Sr	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	121 - 138 no										
55 Cs	56 Ba	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 X?	112 X?	139 no	140 no	141 no	142 no	143 no	144 no	145 no	146 no	147 no	148 no	149 no	150 no	151 no	152 no	...										
87 Fr	88 Ra	113 X?	114 X?	115 X?	116 X?	117 no	118 no	153 no	154 no	155 no	156 no	157 no	158 no	159 no	160 no	161 no	162 no	...	...																							
...	...																																									

Fig. 11. The inhabitants of Mendeleev city. The family of halogens (with an infinite number of elements) corresponds to  $(\ell = 1, j = \frac{3}{2}, m = \frac{1}{2})$  and  $n = 2, 3, 4, \dots$ .

1 H	2 He																																									
3 Li	4 Be	5 B	6 C	7 N	8 O	9 F	10 Ne																																			
11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn																									
19 K	20 Ca	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb											
37 Rb	38 Sr	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	121 - 138 no										
55 Cs	56 Ba	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 X?	112 X?	139 no	140 no	141 no	142 no	143 no	144 no	145 no	146 no	147 no	148 no	149 no	150 no	151 no	152 no	...										
87 Fr	88 Ra	113 X?	114 X?	115 X?	116 X?	117 no	118 no	153 no	154 no	155 no	156 no	157 no	158 no	159 no	160 no	161 no	162 no	...																								
...	...																															...										

Fig. 12. The inhabitants of Mendeleev city. The family of noble gases (with an infinite number of elements) corresponds to  $(\ell = 1, j = \frac{3}{2}, m = \frac{3}{2})$  and  $n = 2, 3, 4, \dots$ .

1 2 H He																			
3 4 Li Be		5 6 B C		7 8 9 10 N O F Ne															
11 12 Na Mg		13 14 Al Si		15 16 17 18 P S Cl Ar		21 22 23 24 Sc Ti V Cr		25 26 27 28 29 30 Mn Fe Co Ni Cu Zn											
19 20 K Ca		31 32 Ga Ge		33 34 35 36 As Se Br Kr		39 40 41 42 Y Zr Nb Mo		43 44 45 46 47 48 Tc Ru Rh Pd Ag Cd		57 58 59 60 61 62 La Ce Pr Nd Pm Sm		63 64 65 66 67 68 69 70 Eu Gd Tb Dy Ho Er Tm Yb							
37 38 Rb Sr		49 50 In Sn		51 52 53 54 Sb Te I Xe		71 72 73 74 Lu Hf Ta W		75 76 77 78 79 80 Re Os Ir Pt Au Hg		89 90 91 92 93 94 Ac Th Pa U Np Pu		95 96 97 98 99 100 101 102 Am Cm Bk Cf Es Fm Md No		121 - 138 no					
55 56 Cs Ba		81 82 Tl Pb		83 84 85 86 Bi Po At Rn		103 104 105 106 Lr Rf Db Sg		107 108 109 110 111 112 Bh Hs Mt Ds X? X?		139 140 141 142 143 144 no no no no no no		145 146 147 148 149 150 151 152 no no no no no no no no		...					
87 88 Fr Ra		113 114 X? X?		115 116 117 118 X? X? no no		153 154 155 156 no no no no		157 158 159 160 161 162 no no no no no no no		...		...							
...																			
...																			

Fig. 13. The inhabitants of Mendeleev city. The three transition series: the iron group series [from Sc(21) to Zn(30)], the palladium group series [from Y(39) to Cd(48)], and the platinum group series [from Lu(71) to Hg(80)].

1 H	2 He																																								
3 Li	4 Be	5 B	6 C	7 N	8 O	9 F	10 Ne																																		
11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn																								
19 K	20 Ca	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb										
37 Rb	38 Sr	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	121 - 138 no									
55 Cs	56 Ba	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 X?	112 X?	139 no	140 no	141 no	142 no	143 no	144 no	145 no	146 no	147 no	148 no	149 no	150 no	151 no	152 no	...									
87 Fr	88 Ra	113 X?	114 X?	115 X?	116 X?	117 no	118 no	153 no	154 no	155 no	156 no	157 no	158 no	159 no	160 no	161 no	162 no	...																							

Fig. 14. The inhabitants of Mendeleev city. The three inner transition series: the lanthanide series [from La(57) to Yb(70)], the actinide series [from Ac(89) to No(102)], and the superactinides series [from (139) to (152)].

1 H	2 He																																								
3 Li	4 Be	5 B	6 C	7 N	8 O	9 F	10 Ne																																		
11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn																								
19 K	20 Ca	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb										
37 Rb	38 Sr	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	121 - 138 no									
55 Cs	56 Ba	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	103 Lr	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 X?	112 X?	139 no	140 no	141 no	142 no	143 no	144 no	145 no	146 no	147 no	148 no	149 no	150 no	151 no	152 no	...									
87 Fr	88 Ra	113 X?	114 X?	115 X?	116 X?	117 no	118 no	153 no	154 no	155 no	156 no	157 no	158 no	159 no	160 no	161 no	162 no	...	...																						
...	...																																								

Fig. 15. The inhabitants of Mendeleev city. The lanthanides or rare earths can be divided into two sub-blocks: the light (or ceric) rare earths [from La(57) to Sm(62)] correspond to  $j = \frac{5}{2}$  and the heavy (or yttric) rare earths [from Eu(63) to Yb(70)] to  $j = \frac{7}{2}$ .

$SO(4, 2)$  part which is a semi-simple Lie group of order  $r = 15$  and of rank  $\ell = 3$ . It has thus fifteen generators involving three Cartan generators (i.e., generators commuting between themselves). Furthermore, it has three invariant operators or Casimir operators (i.e., independent polynomials, in the enveloping algebra of the Lie algebra of  $SO(4, 2)$ , that commute with all generators of the group  $SO(4, 2)$ ). Therefore, we have a set of six  $(3 + 3)$  operators that commute between themselves: the three Cartan generators and the three Casimir operators. Indeed, this set is not complete from the mathematical point of view. In other words, the eigenvalues of the six above-mentioned operators are not sufficient for labelling the state vectors in the representation space of  $SO(4, 2)$ . According to a (not very well-known) result popularised by Racah, we need to find  $\frac{1}{2}(r - 3\ell) = 3$  additional operators in order to complete the set of the six preceding operators. This yields a complete set of nine  $(6 + 3)$  commuting operators and this solves the state labelling problem for the group  $SO(4, 2)$ . The consideration of the group  $SU(2)$  is trivial:  $SU(2)$  is a semi-simple Lie group of order  $r = 3$  and of rank  $\ell = 1$  so that  $\frac{1}{2}(r - 3\ell) = 0$  in that case. As a result, we end up with a complete set of eleven  $(9 + 2)$  commuting operators. It is to be stressed that this result constitutes the key and original starting point of the programme.

The second step establishes contact with chemical physics. Each of the eleven operators can be taken to be self-adjoint and thus, from the quantum-mechanical point of view, can describe an observable. Indeed, four of the eleven operators, namely, the three Casimir operators of  $SO(4, 2)$  and the Casimir operator of  $SU(2)$ , serve for labelling the representation  $h \otimes [2]$  of  $SO(4, 2) \otimes SU(2)$  for which the various chemical elements are partners. The seven remaining operators can thus be used for describing chemical and physical properties of the elements like: ionization energy; oxydation degree; electron affinity; electronegativity; melting and boiling points; specific heat; atomic radius; atomic volume; density; magnetic susceptibility; solubility; etc. In most cases, this can be done by expressing a chemical observable associated with a given property in terms of the seven operators which serve as an integrity basis for the various observables. Each observable can be developed as a linear combination of operators constructed from the integrity basis. This is reminiscent of group-theoretical techniques used in nuclear and atomic spectroscopy (cf. the Interacting Boson Model) or in hadronic spectroscopy (cf. the Gell-Mann/Okubo mass formulas for baryons and mesons).

The last step is to proceed to a diagonalisation process and then to fit the various linear combinations to experimental data. This can be achieved through fitting procedures concerning either a period of elements (taken along a same line of the periodic table) or a family of elements (taken along a same column of the periodic table). For each property this will lead to a formula or phenomenological law that can be used in turn for making predictions concerning the chemical elements for which no data are available. In addition, it is hoped that this will shed light on regularities and well-known (as well as recently discovered) patterns of the periodic table. This programme, referred to as the KGR programme, was briefly presented at the 2003 Harry Wiener International Conference. It is presently under progress.

## 6 Closing remarks

We close this paper with two remarks. Possible extensions of this work concern isotopes and molecules. The consideration of isotopes needs the introduction of the number of nucleons in the atomic nucleus. With such an introduction we have to consider other dimensions for Mendeleev city: the city is not anymore restricted to spread in Flatland. Group-theoretical analyses of periodic systems of molecules can be achieved by considering direct products involving several copies of  $SO(4, 2) \otimes SU(2)$ . Several works have been already devoted to this subject [13].

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